SPECTROSCOPIA MOLECULAR

Un bulletin mensual de novas e informationes de interesse e valor al spectroscopistas molecular

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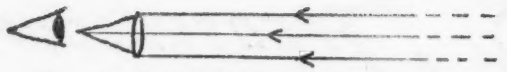
ACCRESCIMENTO SCIENTIFIC es quasi invariabilemente le resultato de fertilisation mutual inter laboratorios e gruppos in partes grandemente separate del mundo. Rarmente recita un homine, o un gruppo de homines, in tonos clar e alte un capitulo integre e importante, o etiam un paragrapho integre e importante, in le epos del scientia. Multo plus frequentemente le comenciamento veni ab alicun voce isolate e forsan timide que face un suggestion inspirate o leva un question stimulante. Iste prime debile voce se reflecte circa le mundo del scientia, le reverberation ab cata laboratorio purificante e fortificante le message, usque finalmente le voce del scientia es decisive e autoritari.

— RAYMOND B. FOSDICK.

NOVE DISVELOPPAMENTOS



**OZONO. Frequentias e intensitates de 191 lineas de absorption de O_3 inter 0 e 11 K (kaysers, cm^{-1}) ha essite calculate. (E. K. GORA, Bul. Am. Phys. Soc. 30, No.3, 66 (1955); Providence College Providence, R. I., Statos Unite.)

* * *

**DISTORTION CENTRIFUGE. Le spectro microundic de O_3 ha essite reanalysate pro includer le effecto del distortion centrifuge. Le deviation median pro 18 lineas esseva ± 1,5 Mc/sec. Le constantes rotational assi obtenite es

A = 106.534,45 Mc/sec,
B = 13.349,10 Mc/sec,
C = 11.834,14 Mc/sec.

(L. PIERCE, ibid., 66; Universitate Harvard, Cambridge, Mass., S. U.)

* * *

**CHLORIDO E BROMIDO DE INDIUM. Spectros rotational de InCl e InBr ha essite observate a alte temperaturas. Distantias internucleari r_e e constantes de interaction de vibration e rotation α_e es

Molecula	r_e (Å)	α_e (Mc/sec)
$In^{115}Cl^{35}$	2,4012±0,0001	15,34±0,15
$In^{115}Br^{69}$	2,5408±0,0001	5,706±0,025
$In^{115}Br^{81}$		5,605±0,018

Le spectros es complicate per le structura hyperfin que resulta ex le interaction de cata momento electric quadrupolic con le campo molecular. Le spectro de $In^{115}Cl^{35}$ da -655±6 Mc/sec e -24±2 Mc/sec como constantes de copula de In^{115} e Cl^{35}, respectivemente. (A. H. BARRETT e M. MANDEL, ibid. 66; Univ. Columbia, New York, N. Y., S. U.)

* * *

**STRUCTURA FIN DE NO_2. Le theoria del structura hyperfin in le spectro microundic de NO_2 ha essite revidite pro includer le caso ubi le interaction de turbination e rotation, e le copula de dipolo con dipolo, es del mesme ordine de magnitude. Le theoria revidite explica satisfacentemente le 10 lineas observate per G. R. Bird (Bul. Am. Phys. Soc. 30, 21 (1955)). Le intensitates predicite del 10 lineas etiam concorda con le observationes intra le errores experimental. (C. C. LIN, ibid. 66; Univ. Harvard.)

* * *

**STATOS TORSIONAL. A causa del torsion interne in CH_3OH, le transition J = 0 → 1 es findite in un serie de duplettos, cata un correspondente a un stato particular de torsion interne. Usate como modello preliminari esseva un rotor symmetric rigide attachate sub un angulo arbitrari a un skeleto asymmetric rigide, e lassate rotar circa su axe de symmetria sub le influentia de un triple barriera de energia potential del typo cosinus. Le Hamiltoniano de isto non explica le findimento de CH_3OH. Nonobstante, un combination semiempiric del formula de Rivelson (J. Chem. Phys. 22, 1733 (1954)) pro le transition correspondente de un rotor symmetric restringite, con elementos de matrice de iste Hamiltoniano, da un bon concordantia con le spectro observate. (P. R. SWAN e M. W. P. STRANDBERG, ibid. 67; Instituto Technologic de Massachusetts, Cambridge, Mass., Statos Unite.)

* * *

**TETRABROMOETHYLENO. Le spectro infrarubie de $Br_2C{=}CBr_2$ ha essite observate e mesurate ab 3 a 100 μ. Iste datos, insimul con le previe spectro Raman e un nove tractamento del coordinatas normal, face possibile pro le prime vice un assignation vibrational que es essentialmente complete e satisfacente. In particular, le fundamentales angular del typos b_{1u}, b_{2u}, e b_{3u} ha essite establite. Le assignationes vibrational de $F_2C{=}CF_2$, $Cl_2C{=}CCl_2$, e $Br_2C{=}CBr_2$ es nunc completemente concorde. (D. E. MANN, J. HAWKINS MEAL, e E. K. PLYLER, ibid. 67; Bureau National de Standards, Washington, D. C., Statos Unite.)

* * *

**MASSAS NUCLEARI EFFICACE. Le contribution electronic a istos in moleculas es discutite. (M. W. P. STRANDBERG, ibid. 67; Instituto Technologic de Massachusetts, Cambridge, Mass., S. U.)

SPECTROS MOLECULAR. III.
TRACTAMENTOS DEL COORDINATAS NORMAL DE MOLECULAS POLYATOMIC
B. APPLICATIONES SPECIFIC

Forrest F. Cleveland, Arnold G. Meister, e Fred L. Voelz
Instituto Technologic de Illinois, Chicago 16, Illinois
(continuate ab Spec. Mol. 4, 30 (1955) - Parcella No.4)

2D. Calculation del Numeros de Undas

HABENTE obtenite le matrices F e G, on pote trovar le numeros de undas σ que corresponde al frequentias fundamental ν como seque. Pro le frequentias del typo a_1, le equation secular in forma expandite es[5]

$$(-\lambda)^2 + (-\lambda)(F_{11}G_{11} + 2F_{12}G_{12} + F_{22}G_{22}) + \begin{vmatrix} F_{11} & F_{12} \\ F_{21} & F_{22} \end{vmatrix} \cdot \begin{vmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{vmatrix} = 0. \qquad (1)$$

Le coefficiente del termino λ es le summa del productos del minores de un linea correspondente del determinantes del matrices F e G, e le termino constante es le producto del determinantes de iste matrices.

A iste puncto il es melior introducer in Eq. 1 le valores numeric del elementos del matrices F e G. Si le constantes del energia potential, distantias ligaminic, e angulos interligaminic es cognoscite, le elementos F_{ij} e G_{ij} del matrices pote esser calculate. Tunc ex Eq. 1 le valores numeric del λ's es obtenite. Finalmente, le numeros de undas σ es calculate ex le relation

$$\sigma = \lambda^{\frac{1}{2}}/2\pi c; \qquad (2)$$

c es le velocitate de lumine (cm/sec).

Pro calcular le numeros de undas, nos usa le sequente valores:[10]

---

[10] Vide G. Glockler, Rev. Modern Phys. 15, 125 (1943).

$\alpha = 104^\circ\ 31'$, $d = 0{,}9580$ Å,

$f_d = 8{,}428$ md/Å, $f_{dd} = -0{,}1051$ md/Å,

$f_\alpha/d^2 = 0{,}7678$ md/Å,

$f_{d\alpha}/d = 0{,}2521$ md/Å.

Ex istos, nos obtene

$$f_\alpha = 0{,}7047 \text{ md Å/rad}^2$$

e

$$f_{d\alpha} = 0{,}2415 \text{ md/rad}.$$

(md = millidynas, Å = angstrom, e rad = radiano.)

Le valores usate pro μ_H e μ_0 esseva

$$\mu_H = (6{,}022 \cdot 10^{23})/1{,}008 = 5{,}974 \cdot 10^{23}\ g^{-1}$$

e

$$\mu_0 = (6{,}022 \cdot 10^{23})/16{,}00 = 3{,}764 \cdot 10^{22}\ g^{-1}.$$

Quando iste valores es usate pro obtener le valores numeric del elementos del matrices F e G, Eq. 1 deveni

$$\lambda^2 - (6{,}159 \cdot 10^{29}\ \text{sec}^{-2})\lambda + 5{,}032 \cdot 10^{58}\ \text{sec}^{-4} = 0. \qquad (3)$$

Ex isto, nos obtene

$$\lambda_1 = 5{,}189 \cdot 10^{29}\ \text{sec}^{-2}$$

$$\lambda_2 = 9{,}700 \cdot 10^{28}\ \text{sec}^{-2}.$$

Substituente iste valores de λ in Eq. 2, e usante $c = 2{,}998 \cdot 10^{10}$ cm/sec, nos obtene

$$\sigma_1 = 3825\ K, \qquad \sigma_2 = 1653\ K.$$[11]

---

[11] Sequente le recommendation del Commission Juncte de Spectroscopia, nos usa σ como le symbolo de numero de undas, e K (kayser) como le unitate correspondente. Vide J. Opt. Soc. Am 43,

410 (1953); Spec. Mol. 3, 67 (1954).

Pro le frequentia ν_3 del typo b_1, le equation secular in forma expandite es multo simple. Illo es

$$\lambda_3 - F_{33} G_{33} = 0. \qquad (4)$$

Iste relation con Eq. 2 da

$$\sigma_3 = (F_{33} G_{33})^{\frac{1}{2}}/(2\pi c). \qquad (5)$$

Usante le constantes previemente date, nos trova que

$$\sigma_3 = 3937 \text{ K}.$$

Le presente valores del numeros de undas es comparate con illos de Dennison[12] in Tabula 2D-1.

TABULA 2D-1. Comparation del presente numeros de undas calculate del molecula H_2O con le valores calculate per Dennison per un methodo differente.

Frequentia vibrational	σ in kaysers	
	Presente valor	Valor de Dennison
$\nu_1(a_1)$	3825	3825,32
$\nu_2(a_1)$	1653	1653,91
$\nu_3(b_1)$	3937	3935,59

---

[12] D. M. Dennison, Rev. Modern Phys. 12 192 (1940).

Eqs. 1 e 5 es naturalmente applicabile a omne molecula nonlinear XY_2, si valores appropriate del constantes es usate.[10]

* * *

ERRORES: In le prime columna de Spec. Mol. 4, 24 (1955) le elemento 13 del 2nde matrice deberea haber essite $2^{\frac{1}{2}}f_{d\alpha}$ (non $2\ f_{d\alpha}$).

Le 3te matrice al mesme pagina deberea haber essite $2^{\frac{1}{2}}f_{d\alpha}$ in le position de F_{12} e F_{21} (non $2\ f_{d\alpha}$).

(Va continuar in un numero futur.)

COMMISSION JUNCTE DE SPECTROSCOPIA

SUB LE EGIDE DEL Consilio International de Uniones Scientific le Commission Juncte de Spectroscopia esseva create per le Union International de Physica Pur e Applicate e per le Union International Astronomic. Le convention al qual le CJS esseva formate occurreva a Cambridge in Anglaterra le 25 al 29 de septembre 1950.

Le 2nde convention esseva tenite a Roma le 9-11 de septembre 1952. Le processo verbal de ille convention esseva publicate in J. Opt. Soc. Am. 43, 410-430 (1953).

Le 3tie convention esseva in Lund in julio 1954. Le processo verbal de isto appareva in Spec. Mol. 3, 67-69 (1954).

Le CJS es componite de 5 representantes ex le UIPPA e 5 ex le UIA. Il ha etiam 2 consilieros, un membro honorari, e un assistente secretario. Dr. William F. Meggers ha essite le chef del CJS depost su fundation.

Le proxime convention del CJS va esser tenite in le Statos Unite in 1956, probabilemente in Columbus, Ohio, al tempore del symposio annual de Ohio State.

CHARLOTTE M. SITTERLY
Bureau National de Standards
Washington 25, D. C., Statos Unite
(Preparate al requesta del redactor.)

K o cm^{-1}; σ o ν ?

UN LITTERA AB Prof. H. H. Nielsen contineva le sequente portion ex le processo verbal del Committee SUN del Union International de Physica Pur e Applicate del qual Dr. Nielsen es le chef:

"(i) Le symbolo pro numero de undas: Le symbolo recommendate per le Commission S.U.N. es σ. Le Union International de Chimia Pur e Applicate recommenda σ tanto como $\tilde{\nu}$.

Post longe discussiones con Dr. Herzberg, qui representava in iste materia le spectroscopistas molecular, il esseva decidite adder a nostre symbolo σ le symbolo $\tilde{\nu}$, con un nota que explica

que iste 2nde indice es usate exclusivemente in spectroscopia molecular."

"(ii) Le nomine kayser pro le unitate cm^{-1}: In le spectroscopia atomic le symbolo K pro cm^{-1} es multo usate a causa del necessitate de exprimer quantitates in millikayser, mK = 0,001 cm^{-1}. Spectroscopistas molecular pare esser contra iste proposition. Proque iste materia pare esser indecise, e proque etiam le Commission Juncte de Spectroscopia non decideva lo a su convention in Lund (julio 1954), il pare consiliabile non prender alicun decisiones in iste respecto ab le latere del Commission S.U.N."

* * *

Le processo verbal del convention in Lund del Commission Juncte de Spectroscopia appareva in Spec. Mol. 3, 67-69 (1954). Le portion que pertine a iste discussion es:

"Le motion de Herzberg pro le retraction del recommendationes concernente kayser e sigma usque un concordantia general esserea attingite recipeva nulle supporto in le CJS. Longe discussiones se disveloppava durante le quales plure resolutiones esseva proponite e rejectate. Finalmente le CJS se decideva a mantener le recommendationes con le sequente emendamentos:

Le symbolo σ debe esser usate pro indicar $1/\lambda_v$ (v = vacuo). Il esseva recognoscite que le UIPPA recommenda $\tilde{\nu}$ como symbolo alternative de numero de undas. Il esseva recognoscite que specialmente in le campo del spectros de moleculas polyatomic il esserea difficile cambiar le ben-establite convention de denotar le numeros de undas vibrational per ν. Quando confusion con frequentia es possibile le uso de $\tilde{\nu}$ o ν' es proponite. Il debe esser sublineate de nove que le recommendationes del CJS non es compulsori."

"De plus, un questionario essera circulate inter un gruppo representative de spectroscopistas pro assecurar lor opiniones in re le symbolo e unitate de numero de undas. Le recommendationes de Roma essera reconsiderate al convention 1956 in le lumine del resultatos del questionario."

* * *

In iste intervallo de indecision, il es necessari que autores e redactores decide qual symbolos illes va usar pro numero de undas.

Il pare clar ab le processos verbal del Committee SUN del UIPPA e del CJS que le symbolo de numero de undas que es preferite per le CJS, le UICPA, e le Committee SUN del UIPPA es σ; e que le altere symbolos alternative es admittite solmente a causa del opposition vigorose de alicun spectroscopistas molecular.

Il etiam es clar que le CJS mantene su recommendation pro K (kayser) como le symbolo e nomine del unitate de numero de undas.

Le symbolo σ etiam ha essite recommendate per le American Association of Physics Teachers e le American Association of Standards (vide Am. J. Phys. 16, 164-179 (1948)); e per le American Society of Mechanical Engineers in su "Letter Symbols for Physics". Iste symbolo etiam esseva usate per Condon e Shortley in lor ben-cognoscite libro super spectros atomic, e in plure articulos super spectros molecular in le J. Chem. Phys.

Certemente, il non pare consiliabile usar symbolos differente in le simile campos de spectros atomic e spectros molecular. Isto causarea multe confusion.

Etiam il non pare sage usar le mesme symbolos pro frequentia e numero de undas; e le symbolo K es certemente plus facile a usar que cm^{-1} o undas per cm.

Consequentemente, il pare melior al redactor de Spec. Mol. usar σ e K como le symbolos de numero de undas e del unitate de numero de undas, respectivemente.[1]

---

[1] Pro previe discussiones de iste materia vide Spec. Mol. 2, 46, 56, 57 (1953); 3, 4, 6, 8, 13, 22, 55, 68 (1954).

Standardisation del symbolos es importante, specialmente pro le novicios in le campo. On spera que spectroscopistas se concordara super le mesme symbolos pro omne brancas de spectroscopia.

NOVE LIBROS

Quantum Mechanics (Mechanica Quantic) F. MANDL. Academic Press, 125 E. 23rd St., New York 10, N. Y.; Butterworths Scientific Publications, London; 1954. 233 + viii paginas. $5.80.

ES DISVELOPPATE LE schema mathematic del theoria del mechanica quantic, sed sin nimie emphase super rigor. Un cognoscentia extense de mathematica non es assumite. Solmente le theoria nonrelativistic es tractate. Le prime 5 capitulos disveloppa in detalio le formalismo mathematic, le sequente 4 tracta del applicationes specific. Le ultime capitulo es un introduction al methodos del theoria de gruppos. Isto es un tractamento simple e systematic del aspectos formal del mechanica quantic e del technicas mathematic usate in su application.

* * *

Elements of Statistical Mechanics (Elementos de Mechanica Statistic). D. ter HAAR. Rinehart and Company, 232 Madison Ave., New York 16, N. Y.; 1954. 468 + xix paginas. $8.50.

UN TRACTAMENTO DEL elementos principal del mechanica statistic, comenciante con le distribution Maxwell e terminante con ensembles de mechanica quantic, con un conto de un numero de applicationes.

* * *

An Outline of Atomic Physics (Elementos de Physica Atomic). O.H. BLACKWOOD, T. H. OSGOOD, e A. E. RUARK. John Wiley and Sons, 440 4th Ave., New York 16, N. Y.; Chapman and Hall, London; 1955. 501 + x paginas. $7.50. 3te edition.

PRO LECTORES QUI HA UN cognoscentia elementari de physica. Tractate es le structura de atomos e moleculas e le natura de radiation. Plus que 35 pro cento del libro es nove. Includite es plure nove problemas e discussiones moderne de tal themas como mesones, resonantia magnetic nucleari, radiation resonantic, spectros Raman, susceptibilitate magnetic, e electrones in metallos. Le libro es un tractamento del significantia del bases fundamental de physica atomic e nucleari.

SUMMARIOS DE ARTICULOS RECENTE

Un Parve Spectrometro de Grilliage Pro Le Region Infrarubie Remote. E. K. PLYLER e N. ACQUISTA. Bureau National de Standards, Washington 25, D. C. J. Chem. Phys. 23, 752 (1955).

IL NUNC ES POSSIBILE mesurar spectros con un prisma de CsI usque a 50 μ.[1] Ultra iste puncto ($\lambda > 50$ μ), un parve grilliage esseva introducite in le spectrometro in loco del reflector Littrow, e con le prisma removite.

Disponibile esseva 2 grilliages, con 320/2,54 e 180/2,54 lineas/cm. Le lineas coperiva un area con lateres de 2,25(2,54) e 3(2,54) cm. Un thermocopula con un fenestra de CsI esseva usabile a 56 μ, e ab 50 a 125 μ un altere con un fenestra de quarz crystallin esseva usate.

Le radiation se originava in un Globar, e le amplificator esseva lo usate in le infrarubio proxime.

Le instrumento esseva probate e calibrate per uso del spectro de H_2O gasose ab 25 a 125 μ. Le 5 lineas proxime a 395 K esseva ben resolvite. Le vapor de H_2O debe esser removite durante le obtention de altere spectros.

Altere grilliages pote esser usate pro obtener le melior resolution in un region particular. A 125 μ, un grilliage de 120/2,54 a 150/2,54 lineas/cm es le optime; e inter 50 e 100 μ, un con circa 240/2,54 lineas/cm es requirite.

[1] N. Acquista e E. K. Plyler, J. Opt. Soc. Am. 43, 977 (1953).

REVISTAS

Theoria Quantic, Theoria de Structura Molecular, e Valentia. J. LENNARD-JONES Ann. Rev. Phys. Chem. 4, 167-188(1953). Departimento de Chimia Theoric, Universitate Cambridge, Anglaterra.

LE THEORIA QUANTIC ha providite con bon successo un comprehension del structura molecular e un description qualitative del proprietates de molecu-

(sequente pagina)

INSTITUTO DE SPECTROSCOPIA INFRARUBIE

UNIVERSITATE FISK va tener su 6te Instituto Annual de Spectroscopia Infrarubie ab le 29 de augusto al 2 de septembre 1955. Isto es destinate a introducer chimistas, biologistas, physicos, e ingenieros al utilitate del spectroscopia infrarubie in le recerca industrial e academic, e in le inseniamento.

Le facultate es: Dr. R. C. Gore, American Cyanamid Company; Dr. A. Nielsen, Universitate Tennessee; Dr. A.L. Smith, Dow-Corning Company; Dr. N. Fuson, Universitate Fisk; Dr. E. Jones, Universitate Vanderbilt; e Dr. J. Lawson, Universitate Statal Tennessee A and I.

Pro plus information tanto como formularios de application, scribe a: Dr. Nelson Fuson, Instituto de Spectroscopia Infrarubie, Universitate Fisk, Nashville, Tenn., Statos Unite.

REVISTAS, continuate ab pagina 40 ...

las. Forsan su plus grand successo de iste typo ha essite le elucidation del proprietates de moleculas conjugate. Del altere latere, le progresso in calculationes quantitative non ha essite si satisfacente. Pro iste ration, attention accrescente ha recentemente essite dirigite al principios fundamental del subjecto pro discoperir ubi meliorationes de un typo basic es possibile. Iste revista da alicun conto de labor de iste typo, tanto como de alicun recente applicationes de existente methodos approximative.

Il ha 3 sectiones principal:

1) Un discussion de theorias currente de structura molecular,

2) un conto de alicun applicationes recente a problemas particular, e

3) un revista de alicunes del difficultates del theoria e un explication in terminos physic del origine de istos.

N O V A S

DR. JOSEPH BOMSTEIN propone que un connexion debe exister inter le COBLENTZ SOCIETY e Spectroscopia Molecular. Le objectivo del societate es servir le spectroscopistas infrarubie; lo del periodico es servir le spectroscopistas molecular. Certemente iste objectivos non es contradictori. Forsan alicun forma de cooperation poterea esser mutualmente avantagiose.

* * *

DR. BOWLING BARNES recipeva le Beckman Award in Chemical Instrumentation al Convention del Societate Chimic American in Cincinnati. Ille es le prime recipiente de iste honor.

* * *

SOROR MIRIAM MICHAEL STIMSON, Chef del Division de Scientia Natural al Collegio Siena Heights, Adrian, Mich., ha recipite ab le American Cancer Society un subvention de $2268 pro le studio del effecto de irradiation ultraviolette super purinos e pyrimidinos in tanto que determinate per le spectros infrarubie.

* * *

UN SPECTROSCOPISTA MICROUNDIC con 20 publicationes in iste campo desira un position a comenciar in septembre 1955. Si vos ha un tal vacantia, scribe a iste periodico, cassa MMDU.

* * *

DRS. F. A. MATSEN e G. R. BIRD ha recipite subventiones pro un intervallo de 3 annos ab le Fundation Welch. Dr. Matsen recipeva $20,000 per anno pro calculationes quanto-méchanic in re le stabilitate e configuration de atomos. Dr. Bird recipeva $4500 per anno pro recerca in spectroscopia microundic.

* * *

DR. A. A. FROST del Universitate Northwestern in Evanston, Illinois, ha recipite un subvention de $10,000 ab le statounitese Fundation National de Scientia pro le studio de energias molecular potential.

* * *

IE LABORATORIO DE SPECTROSCOPIA in le Departimento de Physica al Instituto Technologic de Illinois ha recipite un subvention ab le Research Corporation pro un anno ($2,000) e un altere ab le statounitese Fundation National de Scientia pro 2 annos ($6,750 per anno) pro recerca super spectros Raman e infrarubie, constantes del energia potential, e proprietates thermodynamic calculate de moleculas polyatomic.

Junio 13-17. 10me symposio annual super spectroscopia e structura molecular. (H. H. Nielsen, Departimento de Physica, Universitate Ohio State, Columbus 10, Ohio, Statos Unite.)

Julio 7-11. Convention de Spectroscopistas Molecular Europee, Oxford, Anglaterra. Spectroscopia ultraviolette absorptionic, Raman e infrarubie includente nove disveloppamentos in tecnicas, spectros vibrational de moleculas complexe, mesurationes con alte resolution, spectros de flammas, campos de fortia, spectros de crystallos, e le infrarubie remote. (H. W. Thompson, St. John's College, Oxford, Anglaterra.)

Julio 18-29. Programma intensive de spectroscopia infrarubie. (R. C. Lord, Laboratorio de Spectroscopia, Instituto Technologic de Massachusetts, Cambridge Massachusetts, Statos Unite.)

Augusto 29 - Septembre 2. 6te Instituto Annual de Spectroscopia Infrarubie al Universitate Fisk. Designate pro introducer al chimistas, biologistas, physicos, e ingenieros le utilitate del spectroscopia infrarubie in le recerca industrial e academic, tanto como in le inseniamento. (N. Fuson, Universitate Fisk, Nashville, Tenn., Statos Unite.)

Septembre 14-16. 2nde symposio Ottawa super spectroscopia applicate. (J. K. Hurwitz, Branca de Minas, 568 Booth St. Ottawa, Ontario, Canada.)

Autumno. 6te Colloquio International de Spectroscopia Applicate, in Hollanda. (C. J. Bakker, Secretario, Commission Juncte de Spectroscopia, Laboratorio Zeeman, Muidergracht 4, Amsterdam C, Hollanda.

Junio 1956. Convention del Commission Juncte pro Spectroscopia. Columbus,Ohio o Washington, D. C., S.U. (W. F. Meggers, Bureau National de Standards, Washington 25, D. C., Statos Unite.)

STATISTICA VITAL

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SPECTROSCOPIA MOLECULAR es redigite e publicate mensualmente in Interlingua per Prof. Forrest F. Cleveland, Laboratorio de Spectroscopia, Instituto Technologic de Illinois, Chicago 16, Illinois, Statos Unite. Manuscriptos pro publication debe esser submittite illac.

Le texto original es legite per Dr. Alexander Gode,Chef del Division de Interlingua de Science Service (80 East 11th St., New York 3, N.Y.) Libros importante super Interlingua, disponibile ab ille adresse, es Interlingua-English Dictionary, Interlingua Grammar, e Interlingua A Prime Vista.

Labor editorial es gratis.Le costo de preparation e distribution es recipite ab spectroscopistas, bibliothecas, e companias. Assistentes de publication es Stta. Ruth Grining e Sr. Jerome M. Dowling. Le imprimer es facite per le Servicios de Bureau sub le direction de Stta. Virginia Brown.

DISPONIBILE

1. Spectroscopia Molecular, 12 numeros per anno, $2.00 nette, franc de posta.
2. Volumines passate de Spec. Mol. pro le annos 1952, 1953, e 1954; $3.00 nette per cata un, franc de posta.
3. Numeros individual, $0.25 per cata un.
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Determination of ORGANIC STRUCTURES by PHYSICAL METHODS

Edited by E. A. BRAUDE
Imperial College of Science and Technology, London

and F. C. NACHOD
Sterling-Winthrop Research Institute, Rensselaer, New York

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During the last three decades a closer liaison between physical and organic chemists has brought about new concepts on chemical structure. Many excellent descriptions of the physical methods are now available, but a critical evaluation of the operational rather than the methodological concept has been lacking. The present work is designed to fill this gap; it deals with the more important physical methods of determining the structure of organic compounds from the functional point of view.

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- Durable silver- and rhodium-plated brass prism
- Sample sizes from 3/8" to 5" square
- Sample thicknesses up to 1/2"

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- Qualitative analysis and infrared specular reflectivity measurements for thick materials
- Qualitative analysis and thickness measurements of thin, metal-backed organic coatings

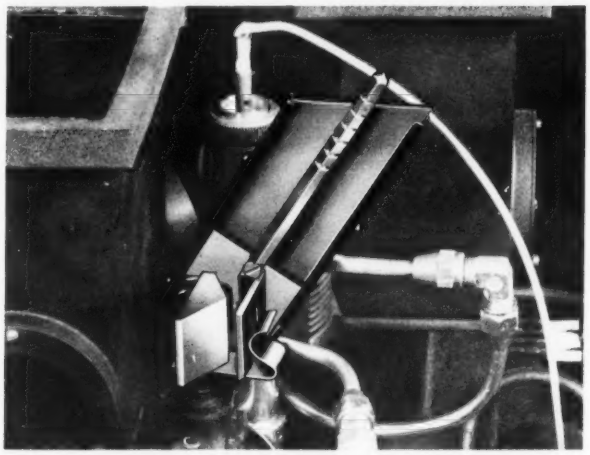

Fig. 1. The Model HT-1 Reflectivity Attachment, as mounted in micro-cell track near globar.

GENERAL DESCRIPTION

The Baird Associates Model HT-1 Reflectance Attachment is an accessory for Models AB and GY Spectrophotometers. This attachment can be used for running the specular reflection curves of any thick material, or the absorption spectra of thin organic coatings on a metallic backing. The attachment fits into the standard Baird Associates micro-cell mounting bracket, which is located near the globar radiation source. No adjustments of sample or attachment are necessary after installation.

The attachment is composed of a reflecting prism, sample holder, and handle, all fastened to a base plate. Base plate and handle are constructed of stainless steel. The prism is cut from brass and plated with silver and rhodium. This rugged scratch- and acid-resistant construction minimizes damage and wear due to handling. The sample holder consists of a slotted stainless steel bracket, backed by a chromium-plated clamping spring. The bracket is machined flat for accurate alignment of the sample surface.

The Baird Associates reflectance attachment is used with nominally flat samples. Minimum sample size of 3/8" x 3/8" (1 cm^2) is determined by the slot width in the sample bracket. Maximum sample size of 5" x 5" is determined by the size of the access hole in the instrument cover. In such sizes, measurements are made only near the corners of the sample. Sample thickness can vary from tissue-thin materials to approximately 1/2". For additional support of thin samples, a backing plate is often used.

Baird Associates wishes to acknowledge the early development work in reflectance measurements by users of the Baird Associates Infrared Spectrophotometer. Special thanks are due Dr. Alex Presnell of the Andrew Jergens Company and Dr. Boyd Hudson, Jr., of Esso Research & Engineering Company.

33 University Road Cambridge 38, Mass., U. S. A.

TECHNICAL INFORMATION

The new Baird Associates Model HT-1 Reflectance Attachment provides a means of obtaining either specular reflection or transmittance curves, depending on sample thickness. In general, samples thinner than 0.001" produce a transmittance curve. Organic materials thicker than 0.1" are generally opaque in the region tested and give a true reflection spectrum.

Optical System: The optical system of the Model HT-1 attachment is illustrated in Fig. 1. The sample beam from the globar passes through a slot in the base plate and reflects off the prism onto the sample surface. Light leaving the sample surface strikes the second face of the prism and passes onto the source mirror. No focusing elements are used.

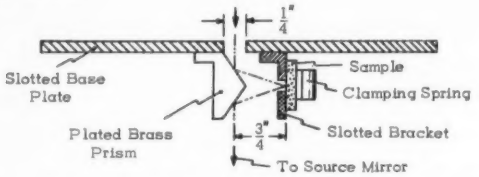

Fig. 2. Optical layout of the Model HT-1 Reflectance Attachment.

Since the rays of the sample beam are extended in going to and from the sample surface, the spectrophotometer entrance slit image is displaced approximately 1 cm toward the source mirror. The effect of this displacement is an approximate 10% shuttering of the sample beam. To balance the sample and reference beams, the same fractional change in the reference beam is achieved by closing the reference beam shutter.

Reflectance Measurements: For reflectance measurements, samples must be nominally flat. Departure from flatness is not critical except where absolute reflectance coefficient measurements are attempted. When the radius of curvature of the test surface is only a few inches, some loss of energy may result and wider slits or slower scanning speeds should be used.

Most nonmetallic materials have a specular reflection in the order of 5 to 20%. The value is particularly low for dull or rough samples, like blotting paper, because of scattering loss. In Baird Associates equipment, however, close proximity of reflection attachment and globar permits measurements of nearly perfect blacks. In such cases, best results are achieved by partial shuttering of the reference beam and the use of wide slits to make up the gain in the instrument servo system. The use of wide slits is permissible since high resolution is not usually necessary to detect reflection bands.

Absolute reflectivity measurements are made by comparing the reflectivity of the sample with the known reflectivity of a standard surface. For absolute reflectivity measurements, it is important that the sample and reference reflectors be as flat as possible and that both sample and reference reflector be accurately aligned against the sample bracket. Where the scattering loss from these reflectors is negligible, comparative measurements of reflectivity can be made accurate to within ±1%.

Transmittance Curves: To obtain transmittance curves for thin organic samples, the sample must have a metallic backing which serves to reflect the energy passing through the sample. A typical curve is illustrated in Fig. 3. In addition to qualitative analysis of the sample, the depth of known bands obtained in this way can be used as a measure of the thickness of the sample. Thick coatings, like most painted surfaces, are opaque and give a reflection rather than a transmittance curve.

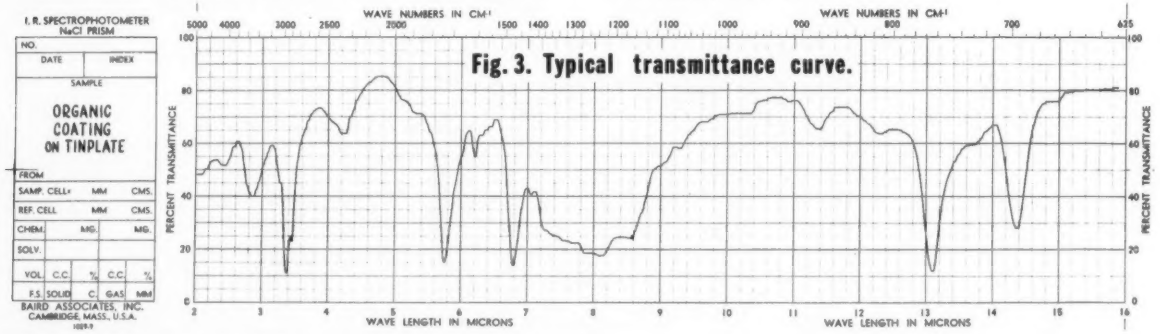

Fig. 3. Typical transmittance curve.

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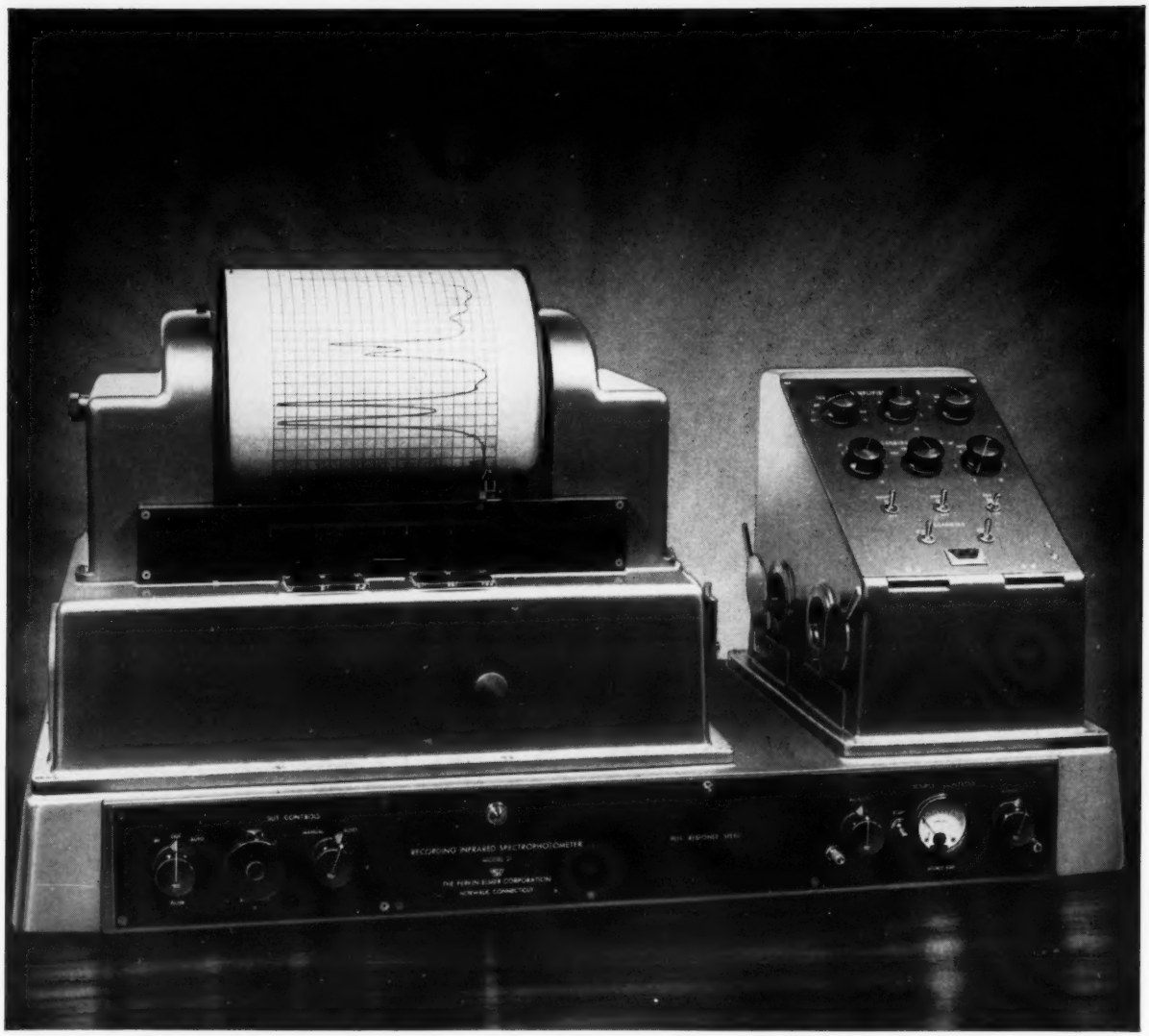

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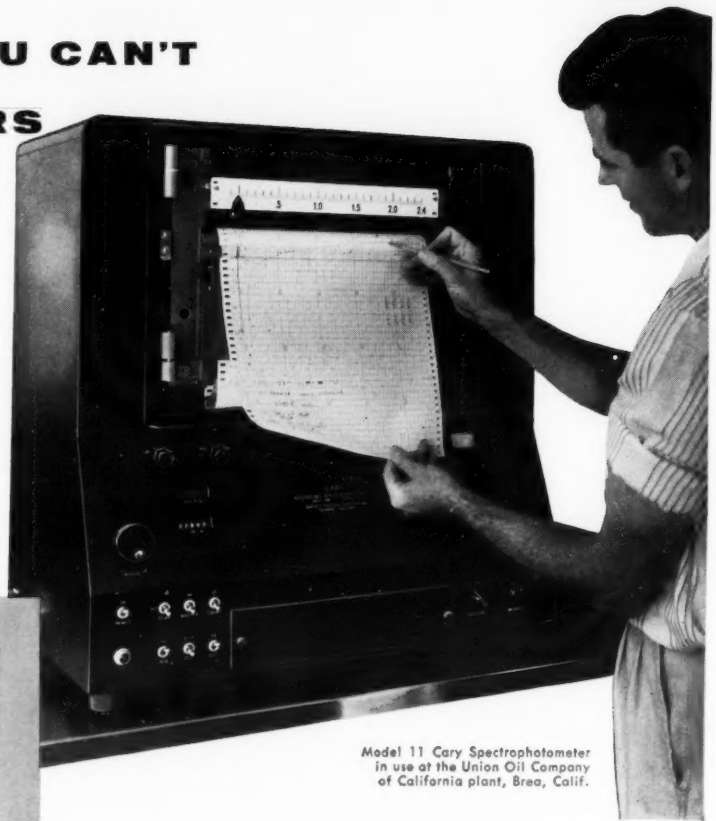

Model 11 Cary Spectrophotometer in use at the Union Oil Company of California plant, Brea, Calif.

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